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Fast iterative solvers

Gerard Sleijpen



Universiteit Utrecht
Department of Mathematics

<http://www.staff.science.uu.nl/~sleij101/>

$$\mathbf{Ax} = \mathbf{b}$$

with \mathbf{A} $n \times n$ non-singular.

Today's topic. Iterative methods for general systems using short recurrences

Program

- CG
- Bi-CG
- Bi-Lanczos
- Hybrid Bi-CG
- Bi-CGSTAB, BiCGstab(ℓ)
- IDR

[Hestenes Stiefel '52]

$\mathbf{A}^* = \mathbf{A} > 0$, Conjugate Gradient

```
 $\mathbf{x} = \mathbf{0}, \mathbf{r} = \mathbf{b}, \mathbf{u} = \mathbf{0}, \rho = 1$   
While  $\|\mathbf{r}\| > tol$  do  
     $\sigma = -\rho, \rho = \mathbf{r}^* \mathbf{r}, \beta = \rho / \sigma$   
     $\mathbf{u} \leftarrow \mathbf{r} - \beta \mathbf{u}, \mathbf{c} = \mathbf{A} \mathbf{u}$   
     $\sigma = \mathbf{u}^* \mathbf{c}, \alpha = \rho / \sigma$   
     $\mathbf{r} \leftarrow \mathbf{r} - \alpha \mathbf{c}$   
     $\mathbf{x} \leftarrow \mathbf{x} + \alpha \mathbf{u}$   
end while
```

Construction CG.

There are three alternative derivations of **CG**.

- **GCR** \rightsquigarrow **CR**,
use \mathbf{A}^{-1} inner product + efficient implementation.
- Lanczos + $T = LU$ + efficient implementation.
- Orthogonalize residuals.

[Ex.8]

Conjugate Gradients, $\mathbf{A}^* = \mathbf{A}$, $\mathbf{K}^* = \mathbf{K}$

$$\begin{aligned} \mathbf{u}_k &= \mathbf{K}^{-1} \mathbf{r}_k - \beta_k \mathbf{u}_{k-1} \\ \mathbf{r}_{k+1} &= \mathbf{r}_k - \alpha_k \mathbf{A} \mathbf{u}_k \end{aligned}$$

Theorem. • $\mathbf{r}_k, \mathbf{K} \mathbf{u}_k \in \mathcal{K}_{k+1}(\mathbf{A} \mathbf{K}^{-1}, \mathbf{r}_0)$

• $\mathbf{r}_0, \dots, \mathbf{r}_{k-1}$ is a **Krylov basis** of $\mathcal{K}_k(\mathbf{A} \mathbf{K}^{-1}, \mathbf{r}_0)$

• If $\mathbf{r}_k, \mathbf{A} \mathbf{u}_k \perp \mathbf{K}^{-1} \mathbf{r}_{k-1}$, then $\mathbf{r}_k, \mathbf{A} \mathbf{u}_k \perp \mathbf{K}^{-1} \mathcal{K}_k(\mathbf{A} \mathbf{K}^{-1}, \mathbf{r}_0)$

Conjugate Gradients, $\mathbf{A}^* = \mathbf{A}$, $\mathbf{K}^* = \mathbf{K}$

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• If $\mathbf{r}_k, \mathbf{A} \mathbf{u}_k \perp \mathbf{K}^{-1} \mathbf{r}_{k-1}$, then $\mathbf{r}_k, \mathbf{A} \mathbf{u}_k \perp \mathbf{K}^{-1} \mathcal{K}_k(\mathbf{A} \mathbf{K}^{-1}, \mathbf{r}_0)$

Proof.

$\mathbf{A} \mathbf{u}_k = \mathbf{A} \mathbf{K}^{-1} \mathbf{r}_k - \beta_k \mathbf{A} \mathbf{u}_{k-1} \perp \mathbf{K}^{-1} \mathbf{r}_{k-1}$ by construction β_{k-1}

$\mathbf{A} \mathbf{u}_k = \mathbf{A} \mathbf{K}^{-1} \mathbf{r}_k - \beta_k \mathbf{A} \mathbf{u}_{k-1} \perp \mathbf{K}^{-1} \mathcal{K}_{k-1}(\mathbf{A} \mathbf{K}^{-1}, \mathbf{r}_0)$ by induction:

$$\begin{aligned} \mathbf{A} \mathbf{K}^{-1} \mathbf{r}_k \perp \mathbf{K}^{-1} \mathcal{K}_{k-1}(\mathbf{A} \mathbf{K}^{-1}, \mathbf{r}_0) &\Leftrightarrow \mathbf{r}_k \perp \mathbf{K}^{-1} \mathbf{A} \mathbf{K}^{-1} \mathcal{K}_{k-1}(\mathbf{A} \mathbf{K}^{-1}, \mathbf{r}_0) \\ &\Leftarrow \mathbf{r}_k \perp \mathbf{K}^{-1} \mathcal{K}_k(\mathbf{A} \mathbf{K}^{-1}, \mathbf{r}_0) \end{aligned}$$

$\mathbf{A}^* = \mathbf{A}$ & $\mathbf{K}^* = \mathbf{K}$: Preconditioned CG

```

x = 0, r = b, u = 0, rho = 1
While ||r|| > tol do
    Solve Kc = r for c
    sigma = -rho, rho = c*r, beta = rho/sigma
    u ← c - beta u, c = Au
    sigma ← u*c, alpha = rho/sigma
    r ← r - alpha c
    x ← x + alpha u
end while
    
```

Properties CG

Pros

- **Low costs per step:** 1 MV, 2 DOT, 3 AXPY to increase dimension Krylov subspace by one.
- **Low storage:** 5 large vectors (incl. \mathbf{b}).
- **Minimal res.** method if \mathbf{A}, \mathbf{K} pos. def.: $\|\mathbf{r}_k\|_{\mathbf{A}^{-1}}$ is min.
- **Orthogonal residual** method if $\mathbf{A}^* = \mathbf{A}, \mathbf{K}^* = \mathbf{K}$:

$$\mathbf{r}_k \perp \mathbf{K}^{-1} \mathcal{K}_k(\mathbf{A}\mathbf{K}^{-1}; \mathbf{r}_0).$$
- No additional knowledge on properties of \mathbf{A} is needed.
- **Robust:** CG always converges if \mathbf{A}, \mathbf{K} pos. def..

Cons

- May **break down** if $\mathbf{A}^* = \mathbf{A} \not\approx 0$.
- Does **not** work if $\mathbf{A} \neq \mathbf{A}^*$.
- CG is sensitive to evaluation errors (often loss of super-linear convergence).

Bi-Conjugate Gradients

$$\begin{aligned} \mathbf{u}_k &= \mathbf{r}_k - \beta_k \mathbf{u}_{k-1} \\ \mathbf{r}_{k+1} &= \mathbf{r}_k - \alpha_k \mathbf{A} \mathbf{u}_k \end{aligned}$$

Theorem. We have $\mathbf{r}_k, \mathbf{u}_k \in \mathcal{K}_{k+1}(\mathbf{A}, \mathbf{r}_0)$.

Suppose $\tilde{\mathbf{r}}_0, \dots, \tilde{\mathbf{r}}_{k-1}$ is a **Krylov basis** of $\mathcal{K}_k(\mathbf{A}^*, \tilde{\mathbf{r}}_0)$.

If $\mathbf{r}_k, \mathbf{A} \mathbf{u}_k \perp \tilde{\mathbf{r}}_{k-1}$, then $\mathbf{r}_k, \mathbf{A} \mathbf{u}_k \perp \mathcal{K}_k(\mathbf{A}^*, \tilde{\mathbf{r}}_0)$.

Proof.

$$\mathbf{r}_k = \mathbf{r}_{k-1} - \alpha_{k-1} \mathbf{A} \mathbf{u}_{k-1} \perp \tilde{\mathbf{r}}_{k-1} \quad \text{by construction } \alpha_{k-1}$$

$$\mathbf{r}_k = \mathbf{r}_{k-1} - \alpha_{k-1} \mathbf{A} \mathbf{u}_{k-1} \perp \mathcal{K}_{k-1}(\mathbf{A}^*, \tilde{\mathbf{r}}_0) \quad \text{by induction}$$

$$\mathbf{A} \mathbf{u}_k = \mathbf{A} \mathbf{r}_k - \beta_k \mathbf{A} \mathbf{u}_{k-1} \perp \tilde{\mathbf{r}}_{k-1} \quad \text{by construction } \beta_{k-1}$$

$$\mathbf{A} \mathbf{u}_k = \mathbf{A} \mathbf{r}_k - \beta_k \mathbf{A} \mathbf{u}_{k-1} \perp \mathcal{K}_{k-1}(\mathbf{A}^*, \tilde{\mathbf{r}}_0) \quad \text{by induction:}$$

$$\mathbf{A} \mathbf{r}_k \perp \mathcal{K}_{k-1}(\mathbf{A}^*, \tilde{\mathbf{r}}_0) \quad \Leftarrow \quad \mathbf{r}_k \perp \mathcal{K}_k(\mathbf{A}^*, \tilde{\mathbf{r}}_0) \supset \mathbf{A}^* \mathcal{K}_{k-1}(\mathbf{A}^*, \tilde{\mathbf{r}}_0)$$

For general square non-singular \mathbf{A}

- Apply **CG** to normal equations ($\mathbf{A}^* \mathbf{A} \mathbf{x} = \mathbf{A}^* \mathbf{b}$) \rightsquigarrow **CGNE**
- Apply **CG** to $\mathbf{A} \mathbf{A}^* \mathbf{y} = \mathbf{b}$ (then $\mathbf{x} = \mathbf{A}^* \mathbf{y}$)
 \rightsquigarrow **Graig's method**

Disadvantage. Search in $\mathcal{K}_k(\mathbf{A}^* \mathbf{A}, \dots)$.

If $\mathbf{A} = \mathbf{A}^*$ then convergence is determined by \mathbf{A}^2 : condition number squared, ...

[Faber Manteufel ']

Theorem. For general square non-singular \mathbf{A} , there is no Krylov solver that finds the best solution in the Krylov subspace $\mathcal{K}_k(\mathbf{A}, \mathbf{r}_0)$ using short recurrences.

Alternative. Construct residuals in a sequence of shrinking spaces (orthogonal to a sequence of growing spaces): adapt the construction of **CG**.

Bi-Conjugate Gradients

$$\begin{aligned} \mathbf{u}_k &= \mathbf{r}_k - \beta_k \mathbf{u}_{k-1} \\ \mathbf{r}_{k+1} &= \mathbf{r}_k - \alpha_k \mathbf{A} \mathbf{u}_k \end{aligned}$$

$$\mathbf{r}_k, \mathbf{u}_k \in \mathcal{K}_{k+1}(\mathbf{A}, \mathbf{r}_0), \quad \mathbf{r}_k, \mathbf{A} \mathbf{u}_k \perp \tilde{\mathbf{r}}_{k-1}$$

With $\rho_k \equiv (\mathbf{r}_k, \tilde{\mathbf{r}}_k)$ & $\sigma_k \equiv (\mathbf{A} \mathbf{u}_k, \tilde{\mathbf{r}}_k)$

and, since $\tilde{\mathbf{r}}_k + \bar{\theta}_k \mathbf{A}^* \tilde{\mathbf{r}}_{k-1} \in \mathcal{K}_k(\mathbf{A}^*, \tilde{\mathbf{r}}_0)$ for some θ_k ,
- is the complex conjugate

we have that
$$\alpha_k = \frac{(\mathbf{r}_k, \tilde{\mathbf{r}}_k)}{(\mathbf{A} \mathbf{u}_k, \tilde{\mathbf{r}}_k)} = \frac{\rho_k}{\sigma_k}$$

and
$$\beta_k = \frac{(\mathbf{A} \mathbf{r}_k, \tilde{\mathbf{r}}_{k-1})}{(\mathbf{A} \mathbf{u}_{k-1}, \tilde{\mathbf{r}}_{k-1})} = \frac{(\mathbf{r}_k, \mathbf{A}^* \tilde{\mathbf{r}}_{k-1})}{\sigma_{k-1}} = \frac{-\rho_k}{\theta_k \sigma_{k-1}}$$

Bi-Conjugate Gradients

$$\begin{aligned} \mathbf{u}_k &= \mathbf{r}_k - \beta_k \mathbf{u}_{k-1} \\ \mathbf{r}_{k+1} &= \mathbf{r}_k - \alpha_k \mathbf{A} \mathbf{u}_k \end{aligned}$$

$$\mathbf{r}_k, \mathbf{u}_k \in \mathcal{K}_{k+1}(\mathbf{A}, \mathbf{r}_0), \quad \mathbf{r}_k, \mathbf{A} \mathbf{u}_k \perp \tilde{\mathbf{r}}_{k-1}$$

With $\rho_k \equiv (\mathbf{r}_k, \bar{q}_k(\mathbf{A}^*) \tilde{\mathbf{r}}_0)$ & $\sigma_k \equiv (\mathbf{A} \mathbf{u}_k, \bar{q}_k(\mathbf{A}^*) \tilde{\mathbf{r}}_0)$
and, since $q_k(\zeta) + \theta_k \zeta q_{k-1}(\zeta) \in \mathcal{P}_{k-1}$ for some θ_k ,

we have that $\alpha_k = \frac{\rho_k}{\sigma_k}$ & $\beta_k = \frac{-\rho_k}{\theta_k \sigma_{k-1}}$

Selecting the initial shadow residual $\tilde{\mathbf{r}}_0$.

- Often recommended: $\tilde{\mathbf{r}}_0 = \mathbf{r}_0$.
- Practical experience: select $\tilde{\mathbf{r}}_0$ randomly.

Exercise. **Bi-CG** and **CG** coincide

if \mathbf{A} is Hermitian and $\tilde{\mathbf{r}}_0 = \mathbf{r}_0$.

Exercise. Derive a version of **Bi-CG** that includes a pre-conditioner \mathbf{K} .

Show that **Bi-CG** and **CG** coincide

if \mathbf{A} and \mathbf{K} are Hermitian and $\tilde{\mathbf{r}}_0 = \mathbf{K}^{-1} \mathbf{r}_0$.

Exercise 8.2 gives an alternative derivation of **Bi-CG**.

Bi-CG

```

 $\mathbf{x} = \mathbf{0}, \mathbf{r} = \mathbf{b}.$  Choose  $\tilde{\mathbf{r}}$ 
 $\mathbf{u} = \mathbf{0}, \rho = 1$   $\tilde{\mathbf{c}} = \mathbf{0}$ 
While  $\|\mathbf{r}\| > tol$  do
   $\sigma = -\rho, \rho = (\mathbf{r}, \tilde{\mathbf{r}}), \beta = \rho/\sigma$ 
   $\mathbf{u} \leftarrow \mathbf{r} - \beta \mathbf{u}, \mathbf{c} \leftarrow \mathbf{A} \mathbf{u},$   $\tilde{\mathbf{c}} \leftarrow \mathbf{A}^* \tilde{\mathbf{r}} - \bar{\beta} \tilde{\mathbf{c}}$ 
   $\sigma = (\mathbf{c}, \tilde{\mathbf{r}}), \alpha = \rho/\sigma$ 
   $\mathbf{r} \leftarrow \mathbf{r} - \alpha \mathbf{c},$   $\tilde{\mathbf{r}} \leftarrow \tilde{\mathbf{r}} - \bar{\alpha} \tilde{\mathbf{c}}$ 
   $\mathbf{x} \leftarrow \mathbf{x} + \alpha \mathbf{u}$ 
end while

```

Properties Bi-CG

Pros

- Usually selects good approximations from the search subspaces (Krylov subspaces).
- **Low costs per step:** 2 DOT, 5 AXPY.
- **Low storage:** 7 large vectors.
- No knowledge on properties of \mathbf{A} is needed.

Cons

- Non-optimal Krylov subspace method.
- Not robust: **Bi-CG** may break down.
- **Bi-CG** is **sensitive to evaluation errors** (often loss of super-linear convergence).
- Convergence depends on **shadow** residual $\tilde{\mathbf{r}}_0$.
- **2 MV needed to expand search subspace by 1 vector.**
- **1 MV is by \mathbf{A}^* .**

Bi-Lanczos

Find coefficients $\alpha_k, \beta_k, \tilde{\alpha}_k$ and $\tilde{\beta}_k$ such that (**bi-orthogonalize**)

$$\gamma_k \mathbf{v}_{k+1} = \mathbf{A} \mathbf{v}_k - \alpha_k \mathbf{v}_k - \beta_k \mathbf{v}_{k-1} - \dots \perp \mathbf{w}_k, \mathbf{w}_{k-1}, \dots$$

$$\tilde{\gamma}_k \mathbf{w}_{k+1} = \mathbf{A}^* \mathbf{w}_k - \tilde{\alpha}_k \mathbf{w}_k - \tilde{\beta}_k \mathbf{w}_{k-1} - \dots \perp \mathbf{v}_k, \mathbf{v}_{k-1}, \dots$$

Select appropriate scaling coefficients γ_k and $\tilde{\gamma}_k$.

Then

$$\mathbf{A} \mathbf{V}_k = \mathbf{V}_{k+1} \underline{H}_k \text{ with } \underline{H}_k \text{ Hessenberg}$$

$$\mathbf{A}^* \mathbf{W}_k = \mathbf{W}_{k+1} \underline{\tilde{H}}_k \text{ with } \underline{\tilde{H}}_k \text{ Hessenberg}$$

$$\text{and } \mathbf{W}_{k+1}^* \mathbf{V}_{k+1} = D_{k+1} \text{ diagonal}$$

Exercise. $T_k \equiv D_k H_k = \underline{\tilde{H}}_k^* D_k$ is tridiagonal.

Exploit $\underline{\tilde{H}}_k = D_k H_k D_k^*$ and tridiagonal structure: **Bi-Lanczos**

Bi-Lanczos

Select a \mathbf{r}_0 , and a $\tilde{\mathbf{r}}_0$
 $\mathbf{v}_1 = \mathbf{r}_0 / \|\mathbf{r}_0\|, \mathbf{v}_0 = \mathbf{0}, \mathbf{w}_1 = \tilde{\mathbf{r}}_0 / \|\tilde{\mathbf{r}}_0\|, \mathbf{w}_0 = \mathbf{0}$
 $\gamma_0 = 0, \delta_0 = 1, \tilde{\gamma}_0 = 0, \tilde{\delta}_0 = 1$
 For $k = 1, 2, \dots$ do
 $\delta_k = \mathbf{w}_k^* \mathbf{v}_k,$
 $\tilde{\mathbf{v}} = \mathbf{A} \mathbf{v}_k, \tilde{\mathbf{w}} = \mathbf{A}^* \mathbf{w}_k$
 $\beta_k = \tilde{\gamma}_{k-1} \delta_k / \delta_{k-1}, \tilde{\beta}_k = \tilde{\gamma}_{k-1} \tilde{\delta}_k / \tilde{\delta}_{k-1}$
 $\tilde{\mathbf{v}} \leftarrow \tilde{\mathbf{v}} - \beta_k \mathbf{v}_{k-1}, \tilde{\mathbf{w}} \leftarrow \tilde{\mathbf{w}} - \tilde{\beta}_k \mathbf{w}_{k-1}$
 $\alpha_k = \mathbf{w}_k^* \tilde{\mathbf{v}} / \delta_k, \tilde{\alpha}_k = \tilde{\mathbf{w}}_k^* \tilde{\mathbf{v}}$
 $\tilde{\mathbf{v}} \leftarrow \tilde{\mathbf{v}} - \alpha_k \mathbf{v}_k, \tilde{\mathbf{w}} \leftarrow \tilde{\mathbf{w}} - \tilde{\alpha}_k \mathbf{w}_k$
 Select a $\gamma_k \neq 0$ and a $\tilde{\gamma}_k \neq 0$
 $\mathbf{v}_{k+1} = \tilde{\mathbf{v}} / \gamma_k, \mathbf{w}_{k+1} = \tilde{\mathbf{w}} / \tilde{\gamma}_k,$
 $\mathbf{V}_k = [\mathbf{V}_{k-1}, \mathbf{v}_k], \mathbf{W}_k = [\mathbf{W}_{k-1}, \mathbf{w}_k]$
 end while

Arnoldi: $\mathbf{A} \mathbf{V}_k = \mathbf{V}_{k+1} \underline{H}_k$.

If $\mathbf{A}^* = \mathbf{A}$, then $\underline{T}_k \equiv \underline{H}_k$ tridiagonal \rightsquigarrow Lanczos

Lanczos + $T = LU$ + efficient implementation \rightsquigarrow CG

Bi-Lanczos + $T = LU$ + efficient implementation \rightsquigarrow Bi-CG

Bi-CG may break down

1) **Bi-Lanczos** may **break down**, i.e., a diagonal element of D_k may be zero. **Lucky** breakdown if $\mathbf{r}_k = \mathbf{0}$.

Corresponds to $\rho = 0$ in **Bi-CG**

Remedie. Look ahead.

2) **Pivot breakdown** or **LU-breakdown**: LU -decomposition may not exist. Corresponds to $\sigma = 0$ in **Bi-CG**

Remedie.

- o Composite step **Bi-CG** (pivot when needed)
- o Form $T = QR$ as in **MINRES** (from the beginning): simple **Quasi Minimal Residuals**

Remedie: o Restart o **QMR**

Note. CG may suffer from pivot breakdown when applied to a Hermitian, non definite matrix ($\mathbf{A}^* = \mathbf{A}$ with positive as well as negative eigenvalues):

MINRES and SYMMLQ cure this breakdown.

Note. Exact breakdowns are rare.

However, near breakdowns lead to irregular convergence and instabilities. This leads to

- o loss of speed of convergence
- o loss of accuracy

Transpose-free Bi-CG

$$\rho_k = (\mathbf{r}_k, \bar{q}_k(\mathbf{A}^*) \tilde{\mathbf{r}}_0) = (q_k(\mathbf{A}) \mathbf{r}_k, \tilde{\mathbf{r}}_0),$$

$$\sigma_k = (\mathbf{A} \mathbf{u}_k, \bar{q}_k(\mathbf{A}^*) \tilde{\mathbf{r}}_0) = (\mathbf{A} q_k(\mathbf{A}) \mathbf{u}_k, \tilde{\mathbf{r}}_0)$$

$$\mathbf{Q}_k \equiv q_k(\mathbf{A})$$

$$(\text{Bi-CG}) \begin{cases} \rho_k, & \mathbf{Q}_k \mathbf{u}_k = \mathbf{Q}_k \mathbf{r}_k - \beta_k \mathbf{Q}_k \mathbf{u}_{k-1}, \\ \sigma_k, & \mathbf{Q}_k \mathbf{r}_{k+1} = \mathbf{Q}_k \mathbf{r}_k - \alpha_k \mathbf{A} \mathbf{Q}_k \mathbf{u}_k, \end{cases}$$

(Pol) Compute q_{k+1} of degree $k+1$ **s.t.** $q_{k+1}(0) = 1$.

Compute $\mathbf{Q}_{k+1} \mathbf{u}_k, \mathbf{Q}_{k+1} \mathbf{r}_{k+1}$

Example. $q_{k+1}(\zeta) = (1 - \omega_k \zeta) q_k(\zeta) \quad (\zeta \in \mathbb{C})$

$$\begin{cases} \omega_k, & \mathbf{Q}_{k+1} \mathbf{u}_k = \mathbf{Q}_k \mathbf{u}_k - \omega_k \mathbf{A} \mathbf{Q}_k \mathbf{u}_k, \\ & \mathbf{Q}_{k+1} \mathbf{r}_{k+1} = \mathbf{Q}_k \mathbf{r}_{k+1} - \omega_k \mathbf{A} \mathbf{Q}_k \mathbf{r}_{k+1}, \end{cases}$$

Transpose-free Bi-CG; Practice

Work with $\mathbf{u}'_k \equiv \mathbf{Q}_k \mathbf{u}_k^{\text{BiCG}}$ and $\mathbf{r}'_k \equiv \mathbf{Q}_k \mathbf{r}_{k+1}^{\text{BiCG}}$

Write \mathbf{u}_{k-1} and \mathbf{r}_k , instead of $\mathbf{Q}_k \mathbf{u}_{k-1}^{\text{BiCG}}$ and $\mathbf{Q}_k \mathbf{r}_k^{\text{BiCG}}$, resp.

$$\rho_k = (\mathbf{r}_k, \tilde{\mathbf{r}}_0), \quad \sigma_k = (\mathbf{A} \mathbf{u}'_k, \tilde{\mathbf{r}}_0)$$

$$(\text{Bi-CG}) \begin{cases} \rho_k = (\mathbf{r}_k, \tilde{\mathbf{r}}_0), & \mathbf{u}'_k = \mathbf{r}_k - \beta_k \mathbf{u}_{k-1}, \\ \sigma_k = (\mathbf{A} \mathbf{u}'_k, \tilde{\mathbf{r}}_0), & \mathbf{r}'_k = \mathbf{r}_k - \alpha_k \mathbf{A} \mathbf{u}'_k, \quad \mathbf{x}'_k = \mathbf{x}_k + \alpha_k \mathbf{u}'_k \end{cases}$$

(Pol) Compute updating coefficients for q_{k+1} .

Compute $\mathbf{u}_k, \mathbf{r}_{k+1}, \mathbf{x}_{k+1}$

Example.

$$\begin{cases} \omega_k, & \mathbf{u}_{k+1} = \mathbf{u}'_k - \omega_k \mathbf{A} \mathbf{u}'_k, \\ & \mathbf{r}_{k+1} = \mathbf{r}'_k - \omega_k \mathbf{A} \mathbf{r}'_k, \quad \mathbf{x}_{k+1} = \mathbf{x}'_k + \omega_k \mathbf{r}'_k \end{cases}$$

Example. $q_{k+1}(\zeta) = (1 - \omega_k \zeta) q_k(\zeta) \quad (\zeta \in \mathbb{C})$

How to choose ω_k ?

Bi-CGSTABILized. With $\mathbf{s}_k \equiv \mathbf{A} \mathbf{r}'_k$,

$$\omega_k \equiv \operatorname{argmin}_{\omega} \|\mathbf{r}'_k - \omega \mathbf{A} \mathbf{r}'_k\|_2 = \frac{\mathbf{s}_k^* \mathbf{r}'_k}{\mathbf{s}_k^* \mathbf{s}_k}.$$

BiCGSTAB

```

x = 0, r = b. Choose  $\tilde{\mathbf{r}}$ 
u = 0,  $\omega = \sigma = 1$ .
While  $\|\mathbf{r}\| > tol$  do
   $\sigma \leftarrow -\omega\sigma$ ,  $\rho = (\mathbf{r}, \tilde{\mathbf{r}})$ ,  $\beta = \rho/\sigma$ 
  u  $\leftarrow$  r -  $\beta$ u, c = Au
   $\sigma = (\mathbf{c}, \tilde{\mathbf{r}})$ ,  $\alpha = \rho/\sigma$ 
  r  $\leftarrow$  r -  $\alpha$ c,
  x  $\leftarrow$  x +  $\alpha$ u
  s = Ar,  $\omega = (\mathbf{r}, \mathbf{s})/(\mathbf{s}, \mathbf{s})$ 
  u  $\leftarrow$  u -  $\omega$ c
  x  $\leftarrow$  x +  $\omega$ r
  r  $\leftarrow$  r -  $\omega$ s
end while

```

Hybrid Bi-CG

Examples.

CGS	Bi-CG \times Bi-CG
Bi-CGSTAB	GCR(1) \times Bi-CG
GPBi-CG	2-truncated GCR \times Bi-CG
BiCGstab(ℓ)	GCR(ℓ) \times Bi-CG

For more details on hybrid Bi-CG, see Exercise 8.12.

For a derivation of GPBi-CG, see Exercise 8.13.

Hybrid Bi-CG or product type Bi-CG

$$\mathbf{r}_k \equiv q_k(\mathbf{A})\mathbf{r}_k^{\text{Bi-CG}} = q_k(\mathbf{A})p_k^{\text{Bi-CG}}(\mathbf{A})\mathbf{r}_0$$

$p_k^{\text{Bi-CG}}$ is the k th “**Bi-CG** residual polynomial”

How to select q_k ??

q_k for **efficient steps** & **fast convergence**.

Fast convergence by

- reducing the residual
- stabilizing the **Bi-CG** part
- other when used as linear solver for the Jacobian system in a Newton scheme for non-linear equations, by reducing the number of Newton steps

Properties hybrid Bi-CG

Pros

- Converges often twice as fast as **Bi-CG** w.r.t. # MVs: each MV expands the search subspace
 - Bi-CG:** $\mathbf{x}_k - \mathbf{x}_0 \in \mathcal{K}_k(\mathbf{A}; \mathbf{r}_0) \hat{=} 2k$ MV.
 - Hybrid **Bi-CG:** $\mathbf{x}_k - \mathbf{x}_0 \in \mathcal{K}_{2k}(\mathbf{A}; \mathbf{r}_0) \hat{=} 2k$ MV.
- Work/MV and storage similar to **Bi-CG**.
- Transpose free.
- Explicit computation of **Bi-CG** scalars.

Cons

- Non-optimal Krylov subspace method.
- Peaks in the convergence history.
- Large intermediate residuals.
- Breakdown possibilities.

Conjugate Gradients Squared

$$\mathbf{r}_k = p_k^{\text{BiCG}}(\mathbf{A}) p_k^{\text{BiCG}}(\mathbf{A}) \mathbf{r}_0$$

CGS exploits recurrence relations for the **Bi-CG** polynomials to design a very efficient algorithm.

Properties

- + Hybrid **Bi-CG**.
- + A very efficient algorithm:
 - 1 DOT/MV, 3.25 AXPY/MV;
 - storage: 7 large vectors.
- Often high peaks in its convergence history
- Often large intermediate residuals
- + Seems to do well as linear solver in a Newton scheme

Properties Bi-CGSTAB

Pros

- Hybrid **Bi-CG**.
- Converges faster (& smoother) than **CGS**.
- More accurate than **CGS**.
- 2 DOT/MV, 3 AXPY/MV.
- Storage: 6 large vectors.

Cons

Danger of

- | | |
|----------------------------|--------------------|
| (A) Lanczos breakdown | $(\rho_k = 0)$, |
| (B) pivot breakdown | $(\sigma_k = 0)$, |
| (C) breakdown minimization | $(\omega_k = 0)$. |

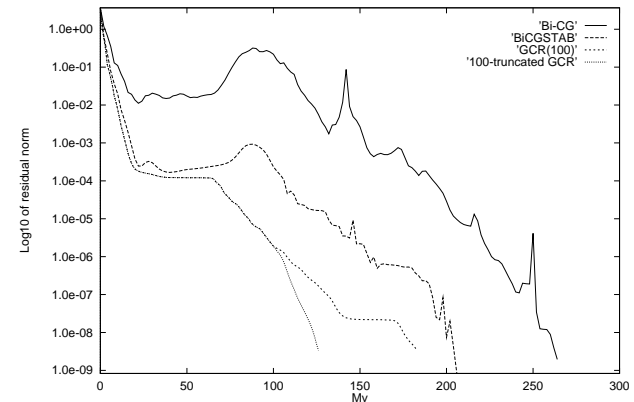
Conjugate Gradients Squared

```

 $\mathbf{x} = \mathbf{0}, \mathbf{r} = \mathbf{b}$ . Choose  $\tilde{\mathbf{r}}$ .
 $\mathbf{u} = \mathbf{w} = \mathbf{0}, \rho = 1$ .

While  $\|\mathbf{r}\| > tol$  do
   $\sigma = -\rho, \rho = (\mathbf{r}, \tilde{\mathbf{r}}), \beta = \rho/\sigma$ 
   $\mathbf{w} \leftarrow \mathbf{u} - \beta \mathbf{w}$ 
   $\mathbf{v} \leftarrow \mathbf{r} - \beta \mathbf{u}$ 
   $\mathbf{w} \leftarrow \mathbf{v} - \beta \mathbf{w}, \mathbf{c} = \mathbf{A}\mathbf{w}$ 
   $\sigma = (\mathbf{c}, \tilde{\mathbf{r}}), \alpha = \rho/\sigma$ 
   $\mathbf{u} = \mathbf{v} - \alpha \mathbf{c}$ 
   $\mathbf{r} \leftarrow \mathbf{r} - \alpha \mathbf{A}(\mathbf{v} + \mathbf{u})$ 
   $\mathbf{x} \leftarrow \mathbf{x} + \alpha(\mathbf{v} + \mathbf{u})$ 
end while

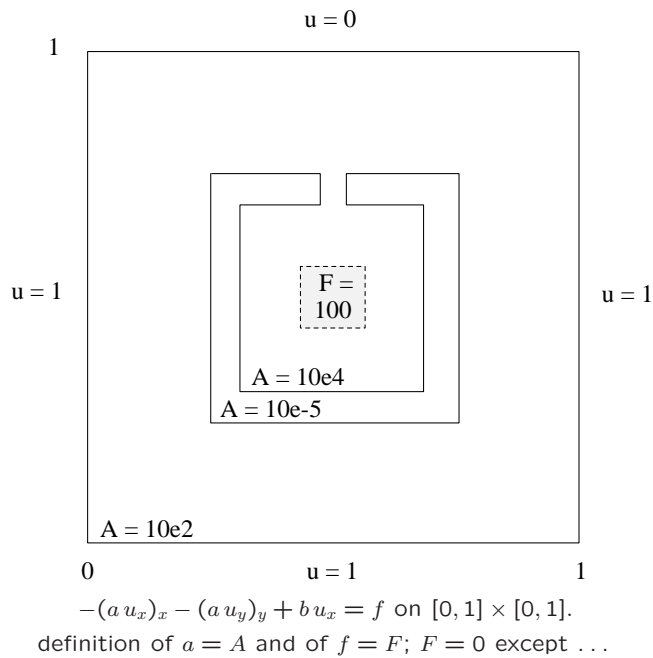
```



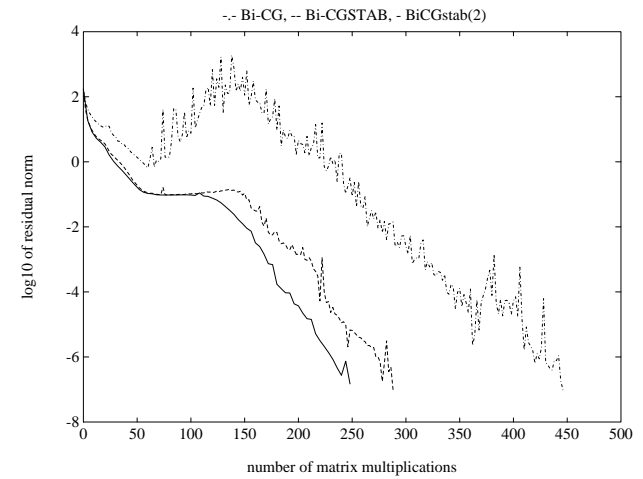
$$-(a u_x)_x - (a u_y)_y = 1 \text{ on } [0, 1] \times [0, 1].$$

$$a = 1000 \text{ for } 0.1 \leq x, y \leq 0.9 \text{ and } a = 1 \text{ elsewhere.}$$

Dirichlet BC on $y = 0$, Neumann BC on other parts of Boundary.
82 × 82 volumes. ILU Decomposition.

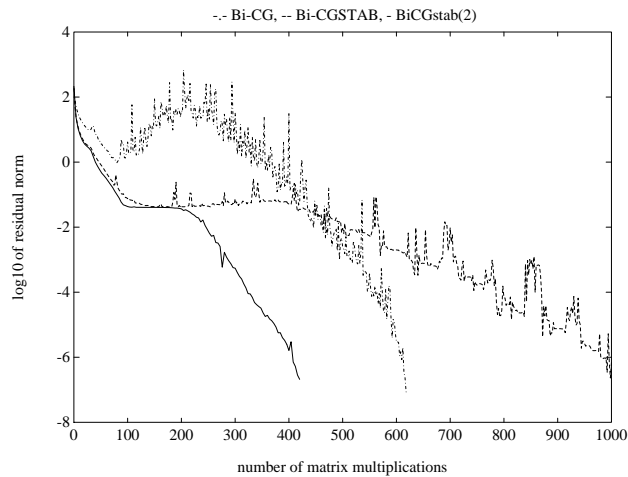


3



$-(a u_x)_x - (a u_y)_y + b u_x = f$ on $[0, 1] \times [0, 1]$.
 $b(x, y) = 2 \exp(2(x^2 + y^2))$, a changes strongly
 Dirichlet BC. 129×129 volumes. ILU Decomp.

3



$-(a u_x)_x - (a u_y)_y + b u_x = f$ on $[0, 1] \times [0, 1]$.
 $b(x, y) = 2 \exp(2(x^2 + y^2))$, a changes strongly
 Dirichlet BC. 201×201 volumes. ILU Decomp.

3

Breakdown of the minimization

Exact arithmetic, $\omega_k = 0$:

— No reduction of residual by

$$\mathbf{Q}_{k+1} r_{k+1} = (\mathbf{I} - \omega_k \mathbf{A}) \mathbf{Q}_k r_{k+1}^{\text{BiCG}} \quad (*)$$

— q_{k+1} is of degree k : **Bi-CG** scalars can not be computed; breakdown of incorporated **Bi-CG**.

Finite precision arithmetic, $\omega_k \approx 0$:

— Poor reduction of residual by (*)

— **Bi-CG** scalars are seriously affected by evaluation errors: drop of speed of convergence.

$\omega_k \approx 0$ to be expected if

A has eigenvalues with rel. large imaginary part: ω_k is real!

Example. $q_{k+1}(\zeta) = (1 - \omega_k \zeta)q_k(\zeta) \quad (\zeta \in \mathbb{C})$.

How to choose ω_k ?

Bi-CGSTABILized. With $\mathbf{s}_k \equiv \mathbf{A}\mathbf{r}'_k$,

$$\omega_k \equiv \operatorname{argmin}_{\omega} \|\mathbf{r}'_k - \omega \mathbf{A}\mathbf{r}'_k\|_2 = \frac{\mathbf{s}_k^* \mathbf{r}'_k}{\mathbf{s}_k^* \mathbf{s}_k} .$$

BiCGstab(ℓ). Cycle ℓ times through the **Bi-CG** part

to compute $\mathbf{A}^j \mathbf{u}'$, $\mathbf{A}^j \mathbf{r}'$ for $j = 0, \dots, \ell$,

where now $\mathbf{u}' \equiv \mathbf{Q}_k \mathbf{u}_{k+\ell-1}^{\text{BiCG}}$ and $\mathbf{r}' \equiv \mathbf{Q}_k \mathbf{r}_{k+\ell}^{\text{BiCG}}$ for $k = m\ell$.

$$\tilde{\gamma}_m \equiv \operatorname{argmin}_{\tilde{\gamma}} \|\mathbf{r}' - [\mathbf{A}\mathbf{r}', \dots, \mathbf{A}^\ell \mathbf{r}'] \tilde{\gamma}\|_2$$

$$\mathbf{r}_{k+\ell} = \mathbf{r}' - [\mathbf{A}\mathbf{r}', \dots, \mathbf{A}^\ell \mathbf{r}'] \tilde{\gamma}_m$$

$$q_{k+\ell}(\zeta) = (1 - [\zeta, \dots, \zeta^\ell] \tilde{\gamma}_m) q_k(\zeta) \quad (\zeta \in \mathbb{C})$$

BiCGstab(ℓ)

```

x = 0, r = [b]. Choose r-tilde.
u = [0], gamma-ell = sigma = 1.
While ||r|| > tol do
    sigma = -gamma-ell * sigma
    For j = 1 to ell do
        rho = (r_j, r-tilde), beta = rho/sigma
        u = r - beta*u, u = [u, Au_j]
        sigma = (u_{j+1}, r-tilde), alpha = rho/sigma
        r = r - alpha*u_{2:j+1}, r = [r, Ar_j]
        x = x + alpha*u_1
    end for
    R = r_{2:ell+1}. Solve (R*R)gamma-tilde = R*r_1 for gamma-tilde
    u = [u_1 - (gamma_1*u_2 + ... + gamma_ell*u_{ell+1})]
    r = [r_1 - (gamma_1*r_2 + ... + gamma_ell*r_{ell+1})]
    x = x + (gamma_1*r_1 + ... + gamma_ell*r_ell)
end while

```

BiCGstab(ℓ) for $\ell \geq 2$ [S1 Fokkema 93, S1 vdV Fokkema 94]

$$\begin{cases} q_{k+1}(\mathbf{A}) = \mathbf{A}q_k(\mathbf{A}) & k \neq m\ell \\ q_{m\ell+l}(\mathbf{A}) = p_m(\mathbf{A})q_{m\ell}(\mathbf{A}) & k = m\ell \end{cases}$$

where p_m of exact degree ℓ , $p_m(0) = 1$ and

$$p_m \text{ minimizes } \|\underbrace{p_m(\mathbf{A}) q_{m\ell}(\mathbf{A}) \mathbf{r}_{m\ell+l}^{\text{BiCG}}}_{\mathbf{r}'}\|_2.$$

p_m **GCR** residual polynomial of degree ℓ

Minimization in practice: $p_m(\zeta) = 1 - \sum_{j=1}^{\ell} \gamma_j^{(m)} \zeta^j$

$$(\gamma_j^{(m)}) \equiv \operatorname{argmin}_{(\gamma_j)} \|\mathbf{r}' - \sum_{j=1}^{\ell} \gamma_j \mathbf{A}^j \mathbf{r}'\|_2,$$

Compute $\mathbf{A}\mathbf{r}'$, $\mathbf{A}^2 \mathbf{r}'$, \dots , $\mathbf{A}^\ell \mathbf{r}'$ explicitly.

With $\mathbf{R} \equiv [\mathbf{A}\mathbf{r}', \dots, \mathbf{A}^\ell \mathbf{r}']$, $\tilde{\gamma}_m \equiv (\gamma_1^{(m)}, \dots, \gamma_\ell^{(m)})^\top$ we have

[Normal Equations, use Choleski] $(\mathbf{R}^* \mathbf{R}) \tilde{\gamma}_m = \mathbf{R}^* \mathbf{r}'$

```

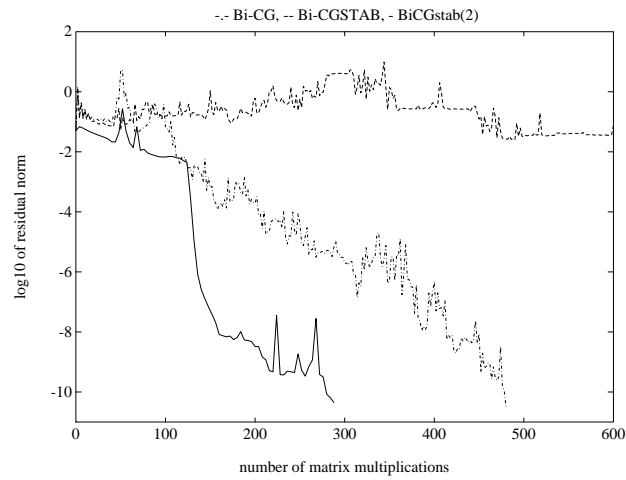
x = zeros(b); rt = rand(b);
sigma = 1; omega = 1; u = zeros(b);
% Computation of initial residual
y = MV(x); r = b-y;

epsilon = 10^(-16); ell = 4;

norm = r'*r; epsilon = norm*epsilon^2; L = 2:ell+1;
while norm > epsilon
    sigma = -omega*sigma; y = r;
    for j = 1:ell
        rho = rt'*y; beta = rho/sigma;
        u = r-beta*u;
        y = MV(u(:,j)); u(:,j+1) = y;
        sigma = rt'*y; alpha = rho/sigma;
        r = r-alpha*u(:,2:j+1);
        x = x+alpha*u(:,1);
        y = MV(r(:,j)); r(:,j+1) = y;
    end

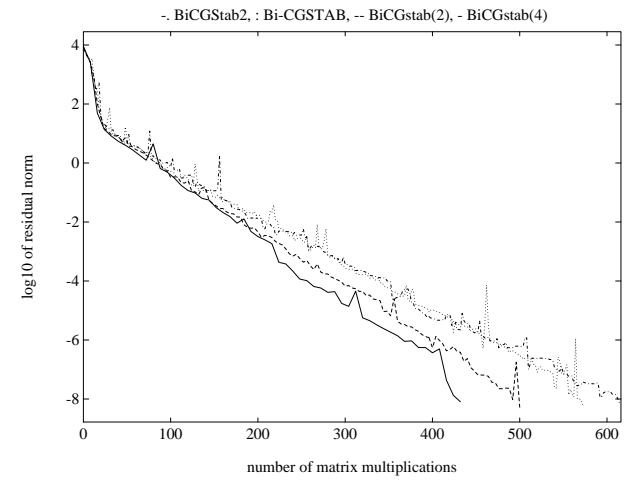
G = r'*r; gamma = G(L,L)\G(L,1); omega = gamma(ell);
u = u*[1;-gamma]; r = r*[1;-gamma]; x = x+r*[gamma;0];
norm = r'*r;
end

```



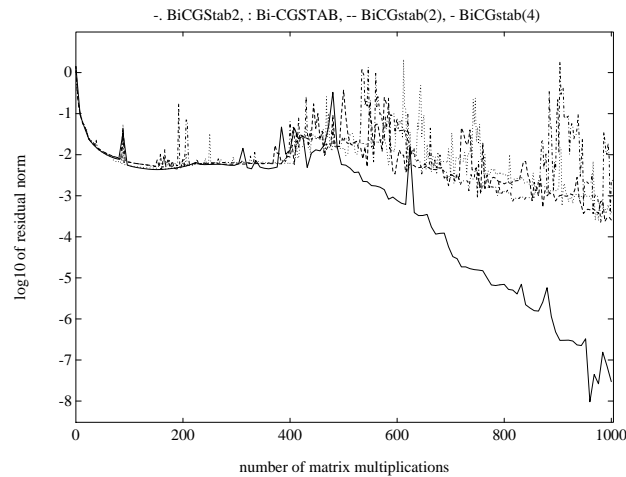
$u_{xx} + u_{yy} + u_{zz} + 1000u_x = f.$
 f s.t. $u(x, y, z) = \exp(xyz) \sin(\pi x) \sin(\pi y) \sin(\pi z).$
 (52 × 52 × 52) volumes. No preconditioning.

4



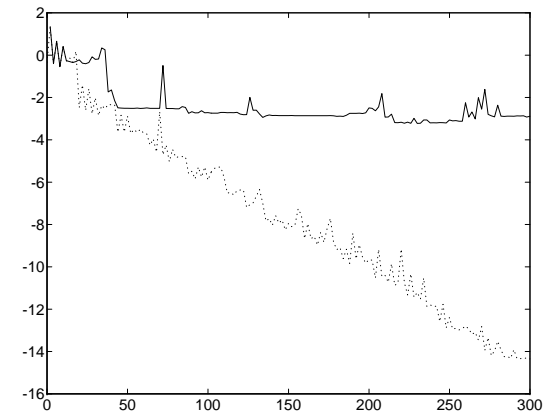
$-(a u_x)_x - (a u_y)_y = 1$ on $[0, 1] \times [0, 1].$
 $a = 1000$ for $0.1 \leq x, y \leq 0.9$ and $a = 1$ elsewhere.
 Dirichlet BC on $y = 0$, Neumann BC on other parts of Boundary.
 200 × 200 volumes. ILU Decomp.

4



$-\epsilon(u_{xx} + u_{yy}) + a(x, y)u_x + b(x, y)u_y = 0$ on $[0, 1] \times [0, 1]$, Dirichlet BC
 $\epsilon = 10^{-1}$, $a(x, y) = 4x(x - 1)(1 - 2y)$, $b(x, y) = 4y(1 - y)(1 - 2x)$,
 $u(x, y) = \sin(\pi x) + \sin(13\pi x) + \sin(\pi y) + \sin(13\pi y)$
 (201 × 201) volumes, no preconditioning.

4



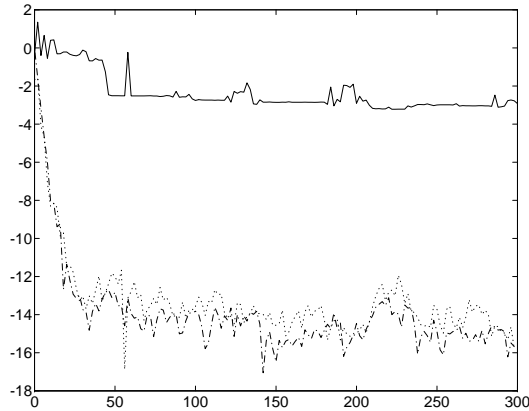
$u_{xx} + u_{yy} + u_{zz} + 1000 u_x = f.$
 f is defined by the solution
 $u(x, y, z) = \exp(xyz) \sin(\pi x) \sin(\pi y) \sin(\pi z).$
 (10 × 10 × 10) volumes. No preconditioning .

4

$$\rho_k = (\mathbf{r}_k, \tilde{\mathbf{r}}_0), \quad \rho_k^* = \rho_k(1 + \epsilon)$$

Accurate Bi-CG coefficients

$$|\epsilon| \leq n \bar{\xi} \frac{\|\mathbf{r}_k\|_2 \|\tilde{\mathbf{r}}_0\|_2}{|(\mathbf{r}_k, \tilde{\mathbf{r}}_0)|} = \frac{n \bar{\xi}}{\hat{\rho}_k} \quad \text{where} \quad \hat{\rho}_k \equiv \frac{|(\mathbf{r}_k, \tilde{\mathbf{r}}_0)|}{\|\mathbf{r}_k\|_2 \|\tilde{\mathbf{r}}_0\|_2}$$



Hybrid Bi-CG

Notation. If p_k is a polynomial of exact degree k , $\tilde{\mathbf{r}}_0$ n -vector, let

$$\mathcal{S}(p_k, \mathbf{A}, \tilde{\mathbf{r}}_0) \equiv \{p_k(\mathbf{A})\mathbf{v} \mid \mathbf{v} \perp \mathcal{K}_k(\mathbf{A}^*, \tilde{\mathbf{r}}_0)\}$$

Theorem. Hybrid **Bi-CG** find residuals $\mathbf{r}_k \in \mathcal{S}(p_k, \mathbf{A}, \tilde{\mathbf{r}}_0)$.

Example.

Bi-CGSTAB: $p_k(\lambda) = (1 - \omega_k \lambda) p_{k-1}(\lambda)$

where, in every step,

$$\omega_k = \text{minarg}_{\omega} \|\mathbf{r} - \omega \mathbf{A} \mathbf{r}\|_2, \quad \text{where } \mathbf{r} = p_{k-1}(\mathbf{A})\mathbf{v}, \quad \mathbf{v} = \mathbf{r}_k^{\text{Bi-CG}}$$

Why using pol. factors of degree ≥ 2 ?

Hybrid **Bi-CG**, that is faster than **Bi-CGSTAB**

1 sweep **BiCGstab**(ℓ) versus ℓ steps **Bi-CGSTAB**:

- Reduction with MR-polynomial of degree ℓ is better than $\ell \times$ MR-pol. of degr. 1.
- MR-polynomial of degree ℓ contributes only once to an increase of $\hat{\rho}_k$

Why not?

- Efficiency:
1.75 + 0.25 · ℓ DOT/MV, 2.5 + 0.5 · ℓ AXPY/MV
Storage: 2 ℓ + 5 large vector.

- Loss of accuracy:

$$\|\mathbf{r}_k\| - \|\mathbf{b} - \mathbf{A}\mathbf{x}_k\| \leq \dots + c \bar{\xi} \max(|\gamma_i|) \|\mathbf{A}\| \|\mathbf{A}^{i-1} \tilde{\mathbf{r}}\|$$

- break-downs are possible

Hybrid Bi-CG

Notation. If p_k is a polynomial of exact degree k , $\tilde{\mathbf{r}}_0$ n -vector, let

$$\mathcal{S}(p_k, \mathbf{A}, \tilde{\mathbf{r}}_0) \equiv \{p_k(\mathbf{A})\mathbf{v} \mid \mathbf{v} \perp \mathcal{K}_k(\mathbf{A}^*, \tilde{\mathbf{r}}_0)\}$$

Theorem. Hybrid **Bi-CG** find residuals $\mathbf{r}_k \in \mathcal{S}(p_k, \mathbf{A}, \tilde{\mathbf{r}}_0)$.

Example.

BiCGstab(ℓ): $p_k(\lambda) = (1 - \omega_k \lambda) p_{k-1}(\lambda)$

where, every ℓ th step

$$\vec{\gamma} = \text{minarg}_{\vec{\gamma}} \|\mathbf{r} - [\mathbf{A}\mathbf{r}, \dots, \mathbf{A}^\ell \mathbf{r}] \vec{\gamma}\|_2, \quad \text{where } \mathbf{r} = p_{k-\ell}(\mathbf{A})\mathbf{r}_k^{\text{Bi-CG}}$$

$$(1 - \gamma_1 \lambda - \dots - \gamma_\ell \lambda^\ell) = (1 - \omega_k \lambda) \cdot \dots \cdot (1 - \omega_{k-\ell} \lambda)$$

Induced Dimension Reduction

Definition. If p_k is a polynomial of exact degree k ,

$\widetilde{\mathbf{R}} \equiv \widetilde{\mathbf{R}}_0 = [\widetilde{\mathbf{r}}_1, \dots, \widetilde{\mathbf{r}}_s]$ an $n \times s$ matrix, then

$$\mathcal{S}(p_k, \mathbf{A}, \widetilde{\mathbf{R}}) \equiv \left\{ p_k(\mathbf{A})\mathbf{v} \mid \mathbf{v} \perp \mathcal{K}_k(\mathbf{A}^*, \widetilde{\mathbf{R}}) \right\},$$

is the p_k -**Sonneveld** subspace. Here

$$\mathcal{K}_k(\mathbf{A}^*, \widetilde{\mathbf{R}}) \equiv \left\{ \sum_{j=0}^{k-1} (\mathbf{A}^*)^j \widetilde{\mathbf{R}} \vec{\gamma}_j \mid \vec{\gamma}_j \in \mathbb{C}^s \right\}.$$

Theorem. IDR find residuals $\mathbf{r}_k \in \mathcal{S}(p_k, \mathbf{A}, \widetilde{\mathbf{R}})$.

Example.

Bi-CGSTAB: $p_k(\lambda) = (1 - \omega_k \lambda) p_{k-1}(\lambda)$

where, in every step,

$\omega_k = \text{minarg}_\omega \|\mathbf{r} - \omega \mathbf{A} \mathbf{r}\|_2$, where $\mathbf{r} = p_{k-1}(\mathbf{A})\mathbf{v}$, $\mathbf{v} = \mathbf{r}_k^{\text{Bi-CG}}$

Select $n \times \ell$ matrices \mathbf{U} and $\widetilde{\mathbf{R}}$

Experiments suggest $\widetilde{\mathbf{R}} = \text{qr}(\text{rand}(n, \ell), 0)$

\mathbf{U} and \mathbf{C} can be constructed from ℓ steps of **GCR**.

IDR

Select an \mathbf{x}_0 .

Select $n \times s$ matrices \mathbf{U} and $\widetilde{\mathbf{R}}$.

Compute $\mathbf{C} \equiv \mathbf{A}\mathbf{U}$.

$\mathbf{x} = \mathbf{x}_0$, $\mathbf{r} = \mathbf{b} - \mathbf{A}\mathbf{x}$, $j = s$, $i = 1$

while $\|\mathbf{r}\| > \text{tol}$ do

Solve $\widetilde{\mathbf{R}}^* \mathbf{C} \vec{\gamma} = \widetilde{\mathbf{R}}^* \mathbf{r}$ for $\vec{\gamma}$

$\mathbf{v} = \mathbf{r} - \mathbf{C} \vec{\gamma}$, $\mathbf{s} = \mathbf{A}\mathbf{v}$

$j++$, if $j > s$, $\omega = \mathbf{s}^* \mathbf{v} / \mathbf{s}^* \mathbf{s}$, $j = 0$

$\mathbf{U} e_i \leftarrow \mathbf{U} \vec{\gamma} + \omega \mathbf{v}$, $\mathbf{x} = \mathbf{x} + \mathbf{U} e_i$

$\mathbf{r}_0 = \mathbf{r}$, $\mathbf{r} = \mathbf{v} - \omega \mathbf{s}$, $\mathbf{C} e_i = \mathbf{r}_0 - \mathbf{r}$

$i++$, if $i > s$, $i = 1$

end while

For more details on IDR, see the Exercises 8.6, 8.14 and 8.15.